N-PHASE INTERFACE TRACKING METHOD UTILIZING
UNIQUE ENUMERATION OF MICROGRID CELLS

TECHNICAL FIELD

This invention relates generally to methods for the simulation of multiphase fluid flows, and more particularly, to those methods which track interfaces between immiscible fluids.

BACKGROUND OF THE INVENTION

The study of interfacial flow is a broad topic of interest in many different research disciplines. Physicists, biologists, engineers and other scientists all share a stake in accurate representation of interfacial position. Whether pipeline flow of crude oil mixtures, cellular disruption or the development of galaxies is to be modeled, interfacial movement intimately influences calculations by accounting for a redistribution of local density functions. In general, the problems of interest have as a common element the requirement to resolve through numerical simulation the complex flow patterns that result from the flow of immiscible (or semi-immiscible) fluids.

Published works dating from the 1960's until now relate an ever-improving understanding of numerical algorithms that allow for an accurate description of interface position. These algorithms are generally categorized as either surface methods or volume methods. However, there is still no generalized method presently developed that allows for the numerical simulation of the dynamic movement of three or more fluid materials and their interfaces.

A reference field or function that moves with an interface typically characterizes surface methods. Sometimes the reference is a mass-less fixed particle along the interface (Daly, 1969; Takizawa et. al, 1992). Other times a level set function which tracks the shortest distance to an interface

1   from a fixed point is offered (Sussman et. al, 1994; Osher and Sethian, 1988;

2   Sethian, 1996). Further references indicate height functions are implemented

3   where a reference line or plane is chosen in the computational domain

4   (Nichols and Hirt, 1973). All of these methods give accurate descriptions of

5   two fluid, single interface problems that do not involve folding, breaking or

6   merging interfaces. The biggest advantage of surface methods is that an

7   interface position is explicitly known for all time.

8

9   Volume methods, however, build a reference within the fluids under

10   evaluation. Typically a method will discretely identify different materials on

11   either side of an interface. Mixed cells then indicate the general location of an

12   interface. An exact location is never discretely known, and volume methods

13   are characterized by a reconstruction step whereby an approximate interface

14   is built from local data consisting of volume and area fractions.

15

16   The volume methods may be further divided into 2 sub-cases to include

17   particle methods and scalar advection methods. Particle methods include the

18   marker and cell (MAC) method (Harlow and Welch, 1965; Daly, 1967) and the

19   particle in cell (PIC) method (Harlow et.al, 1976). These algorithms employ

20   the idea of mass-less particles to identify a particular material and then track

21   their movements through a static grid based on local velocity conditions. The

22   volume of fluid (VOF) method (Hirt and Nichols, 1981; Ashgriz and Poo, 1991;

23   Lafaurie et.al, 1994) and various line techniques including SLIC (Noh and

24   Woodward, 1976), PLIC (Youngs, 1982) and FLAIR (Ashgriz and Poo, 1991)

25   implement several unidirectional sweeps to predict the change in volume

26   fractions of cells at each time step based on a local resolution of the scalar

27   transport equation. There are many combination algorithms presently used

28   which implement both VOF and line techniques to capture even greater

29   interface detail (Rider and Kothe, 1998; Gueyffier et al., 1999; Scardovelli

30   et al., 2000, 2002). Volume methods offer good interfacial descriptions of

31   complicated fluid geometries in both two and three dimensions and allow for

1   interface folding, breaking, and merging. However these methods are

2   restricted to cases involving only two materials.

3

4   Traditional VOF methods define a concentration function, C, to denote

5   materials. Typically,

6     $C = \begin{cases} 1, \text{fluid 1} \\ 0, \text{fluid 2} \end{cases}$

7   where values between 0 and 1 represent mixed cells.

8

9   C is then transported by the velocity field **u** via the scalar transport equation,

10     $\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = 0.$

11

12   And finally, the average (or cell centered) values of density, ρ, and

13   viscosity, μ, are interpolated as: $\rho = C\rho_1 + (1-C)\rho_2$ and $\mu = C\mu_1 + (1-C)\mu_2$

14   where the subscripts 1 and 2 refer to materials 1 and 2. In this interpretation,

15   C, although called a concentration function, acts as the fluid fraction of

16   material 1 or 2 in any given cell.

17

18   Methods have been employed previously which have attempted to track two

19   interfaces or three materials in a computational fluid simulation. These

20   methods (Eulerian-Eulerian) operate by using control volumes which may

21   contain at most three materials and two unique interfaces. As discussed

22   above, at least a single set of conservation equations is still required to

23   resolve the flow field dynamics, i.e., mass conservation equation and two or

24   three momentum conservation equations dependent on the dimensionality of

25   the problem (2D or 3D), or a complete set of conservation equations is solved

26   for each material. However, no one to date has addressed the issue of

27   uniquely identifying and tracking, with a single or multiple concentration

28   function(s) C_i, three or more materials. The issue always distills down to the

29   unique tracking and resolving of multiple interfaces in a computational cell. In

30   addition, when multiple equation sets are used as possibly in Eulerian-

1   Eulerian methods, the numerical problem becomes intractable when folding,

2   breaking, and reforming interfaces exist due to the need to precisely define

3   the interface shape inorder to apply the constitutive relationships between

4   materials in this formulation. The above described computational fluid

5   dynamic methods fail to provide a method which can readily handle explicit or

6   implicit tracking of the interface between three or more generally immiscible

7   fluid materials.   The present invention provides an efficient and tractable

8   method which overcomes the deficiency of current methods in tracking

9   multiple fluid materials and their interfaces.

10

11   **SUMMARY OF THE INVENTION**

12

13   A method for tracking N materials and their interfaces in a computational

14   domain is disclosed. A macrogrid including control volumes is created on a

15   computational domain in which N materials and their interfaces are to be

16   tracked. A microgrid including microgrid cells is overlaid upon the macrogrid

17   with each of the microgrid cells being coupled to a control volume. The

18   macrogrid and control volumes are initialized with initial and boundary

19   conditions representative of the problem to be solved. A unique identifier

20   number is assigned to each of the N materials and to the microgrid cells

21   containing those N materials. Volume fractions for the N-materials in the

22   control volumes can then be calculated. Similarly, average density and

23   average viscosity for each of the control volumes may be discretely

24   determined.

25

26   Equations of fluid motion (the Navier Stokes equations) may then be solved

27   upon the macrogrid and control volumes using the initial and boundary

28   conditions and properties dependent upon the volume fractions, i.e., average

29   density and average viscosity, to arrive at local velocity conditions for the

30   control volumes. The microgrid cells within the microgrid are then advected in

31   response to the calculated local velocity conditions in the control volumes with

32   voids and overlaps of the microcells occurring in the microgrid. The location

1 of each of the advected microcells is tracked using the unique enumeration

2 previously assigned to each of the microgrid cells. Preferably, this unique

3 enumeration includes the use of prime numbers, such as those generated by

4 an Eulerian quadratic number generator.

5

6 Overlapped microgrid cells are then reallocated within the microgrid so that

7 only one microgrid cell is located in each space of the microgrid to effectively

8 conserve mass and satisfy local fluid fraction gradient values. The contents of

9 the microgrid cells can then be used in additional time steps or iterations to

10 determine new values for volume fractions of the fluid materials in the

11 microgrid cells. The equations of fluid motion can then be iteratively solved

12 again using updated properties dependent upon the volume fractions. This

13 process of iteratively determining new fluid fractions in the control volumes,

14 solving equations of fluid motion to arrive at new velocity fields, advecting

15 microcells in accordance with the newly derived velocity fields, and then

16 reallocating the microcells to comport with constraints such as conservation of

17 momentum and conservation of mass is repeated over many time steps to

18 simulate the fluid flow.

19

20 A method for tracking cells in a fluid dynamics computation is now described.

21 Unique identifier numbers are assigned to microgrid cells located in a grid.

22 The unique identifiers are associated with respective N fluid materials. N may

23 be 2 or more materials. Preferably, the unique identifiers are prime numbers,

24 such as those generated by an Eulerian quadratic number generator.

25

26 The cells are advected within a grid in response to local velocity conditions

27 such that some of the cells overlap one another while voids are also created

28 in the grid. Grid locations with overlapped cells are identified by determining

29 that a combination of the unique identifiers coexist in that grid location. The

30 fluid materials of the microgrid cells disposed in a grid location can be

31 determined using modular arithmetic when using unique identifiers which are

32 prime numbers. The cells can then be reallocated to comport with specified

1　conservation of mass and momentum restrictions with one unique identifier

2　again occupying each space in the microgrid. Volume fractions of fluid

3　materials in specific areas of a computational space can then be computed to

4　determine properties, such as average density and average viscosity, which

5　are to be used in a next time step to again solve the time-dependent fluid

6　equations of motion.

7

8　It is an object of the present invention to provide a method for simulating fluid

9　flow that can easily handle two or more generally immiscible fluid materials

10　and track the interfaces between the different materials.

11

12　It is yet another object to provide a method for tracking two or more materials

13　and their associated interfaces based on the creation of elemental pieces or

14　microgrid cells of fluid material and the use of a unique tagging system based

15　on prime numbers.

16

17　It is still yet another object to provide a method for tracking N materials and

18　their associated interfaces by uniquely identifying and tracking, with a single

19　concentration function C, N fluid materials wherein N may be 2 or greater.

20

21　**BRIEF DESCRIPTION OF THE DRAWINGS**

22

23　These and other objects, features and advantages of the present invention

24　will become better understood with regard to the following description,

25　pending claims and accompanying drawings where:

26

27　FIG. 1 is a flowchart of the overall steps taken in modeling the flow of N fluid

28　materials and tracking the interfaces between the fluid materials;

29

30　FIG. 2 illustrates a macrogrid including a macrocell or control volume which is

31　overlayed with a 4 x 4 array of microgrid cells containing one of three distinct

32　fluid materials which are identified by three corresponding prime numbers;

1   FIG. 3A shows a macrogrid including an array of 2 x 2 control volumes with an
2   array of 3 x 3 microgrid cells overlaying each of the control volumes and FIG.
3   3B is a corresponding chart including a matrix of prime numerals
4   corresponding to the materials in the microgrid cells;
5
6   FIG. 4A shows an example of flux handling with prime enumerated microgrid
7   cells showing a microgrid having overlapping cells and voids and FIG 4B is a
8   corresponding chart including a matrix of prime numbers and products of
9   prime numbers corresponding to the materials in the microgrid cells;
10
11   FIGS. 5A and 5B illustrate a visualization of a 2D scanning technique wherein
12   FIG 5A shows a first scan and FIG. 5B shows a second scan which begins at
13   a different starting point than the scan of FIG. 5A;
14
15   FIG. 6 is a flowchart describing steps for reallocating microgrid cells;
16
17   FIG. 7 is a flowchart describing steps in scanning a grid and reallocating
18   microgrid cells into voids found in the microgrid;
19
20   FIG. 8 shows a definition for a theoretical flow in a rectangular cavity in which
21   a plurality of fluid materials is allowed to swirl and mix;
22
23   FIG. 9 is a photographic representation of a test showing the swirl pattern in a
24   rectangular cavity defined in FIG. 8;
25
26   FIGS. 10A and 10B show a shear driven recirculating cavity flow with three
27   distinct numerical layers employing the microgrid algorithm of the present
28   invention;
29
30   FIG. 11 shows a shear driven recirculating cavity flow with 3 distinct numerical
31   layers employing the microgrid algorithm with a 2 x 2 refinement and a
32   comparative 4 x 4 refinement at a time of 210 seconds;

1   FIG. 12 shows a shear driven cavity flow with 6 materials at time steps of 0,

2   120, 240, and 360 seconds utilizing a 8 x 8 microgrid; and

3

4   FIG. 13 shows an artistic rendering of a shear driven cavity flow with 6

5   colocated materials at 120 seconds.

6

7   **BEST MODE FOR CARRYING OUT THE INVENTION**

8

9   The present invention provides a method for simulating the flow of

10   N-immiscible fluid materials and tracking the position of the interfaces

11   between the fluid materials. For the purpose of simplicity, an example utilizing

12   three separate materials will be described. The method may easily be

13   extended to model with a much larger number of fluid materials and

14   interfaces. For example, using a particular number generator (Eulerian

15   quadratic generator) and identification system for fluid materials, 39 materials

16   may be used based on this prime number generator. Through use of other

17   generators of unique identifiers, an even a higher number of materials and

18   interfaces may be tracked.

19

20   An exemplary embodiment of a method for tracking N fluid materials and their

21   interfaces, made in accordance with the present invention, is shown in a

22   flowchart in FIG. 1.

23

24   A first step 110 is to create a macrogrid filled with macrocells or control

25   volumes to define an overall computational space in which the flow of N fluid

26   materials is to be simulated. For example, fluid flow circulating in a

27   rectangular cavity will be described in greater detail below.

28

29   Step 120 includes applying initial and boundary conditions to the macrogrid

30   and control volumes. In this exemplary embodiment, the boundary conditions

31   include no-slip walls and a fixed tangential (or shear) velocity condition on the

32   top surface of the cavity. Initial conditions are quiescent or zero velocity for

1   the fluids with a hydrostatic pressure distribution imposed in the vertical

2   direction due to gravity forcing. Those skilled in the art of computational fluid

3   dynamics modeling and simulation will appreciate that models can be made

4   employing, by way of example and not limitation, other boundary and initial

5   conditions such as symmetry planes, inflow and outflow boundaries, constant

6   pressure surfaces, and an initial mean velocity and density distribution applied

7   to the fluid materials.

8

9   A microgrid filled with microgrid cells is then overlaid upon the macrogrid and

10   control volumes in step 130. FIG. 2 illustrates a single macrocell or control

11   volume which is overlaid with a microgrid including a 4 x 4 array of microcells.

12   In this particular preferred embodiment, all of the microgrid cells are of the

13   same size and shape. The present invention could also be extended to use

14   microgrid cells having different sizes and shapes. Microgrid cells offer a

15   discrete and simple way to delineate materials in a computational space

16   without the complexity of formal interface reconstruction at every time step. In

17   the microcell technique of the present exemplary embodiment of this

18   invention, the resolution of an interface is predetermined by the size of the

19   microgrid cells themselves and no cell by cell reconstruction is necessary.

20

21   N fluid materials are then assigned in step 140 to each of the microgrid cells.

22   In this example, N= 3 as the flow of three fluid materials will be simulated. In

23   FIG. 2, note that the microgrid cells are shaded to depict each of three

24   different fluid materials 1, 2 and 3. As a numerical representation of the

25   physical system is created, a single prime number or identifier associated with

26   a particular fluid material is assigned to each microgrid cell. For example, all

27   microgrid cells that contain material N=1 are given the identifier 43. All

28   microgrid cells that contain material N=2 are assigned the identifier 47 and

29   cells containing material N=3 are labeled with the identifier 53. In this way, a

30   prime representation of the system is built. Prime numbers less than 43 are

31   not used in this exemplary embodiment because of a requirement that the

32   square of any prime number be greater than the largest prime number

1   assigned to a material. This assignment renders the evaluated primes into a

2   mathematically unique set which enhances the tracking of microcells.

3

4   Utilizing the same shading scheme as depicted in FIG. 2, FIG. 3 shows a

5   macrogrid including a 2 x 2 array of control volumes each with a 3 x 3 array of

6   microcells. Assume this is at an initial or first time step or t=0 seconds. The

7   location of each material is accounted for in a microcellular fashion as shown

8   in FIG. 3B utilizing a chart with a corresponding numerical representation of

9   the microgrid cells and their assigned fluid materials.

10

11 A prime number generator is utilized in this preferred embodiment that will

12 create enough unique primes to delineate every material in the simulation.

13 This particular prime number generator has the following characteristics:

14

15   1.   the smallest prime number generated squared is greater than the

16   largest prime number generated; and

17   2.   the generator creates a monotonically increasing set of primes.

18

19 By way of example and not limitation, a good 'all-purpose' generator that has

20 these characteristics, and allows up to N=39 (where N is a positive integer), is

21 the Eulerian quadratic generator, $p(N) = N^2 + N + 41$. By the nature of how an

22 algebraic generator works, some primes may be skipped. This particular

23 generator creates a set of non-inclusive primes from 43 to 1601 as is

24 demonstrated in Table 1. Note that the largest prime generated, 1601, is

25 smaller than the smallest prime generated squared, $43^2 = 1849$.

26

27   Table 1: Prime generator example.

N	$p(N) = N^2 + N + 41$	$p^2(N)$
1	43	1849
2	47	
3	53	

37	1447	
38	1522	
39	1601	
40	1681 (not prime) $= 41^2$	

1

2 In step 150, the volume fractions of the fluid materials in each of the control

3 volumes are calculated. The prime marking technique is employed to resolve

4 the fluid fraction of each material in each control volume. Fluid fraction, f_N,

5 may be recovered as a volume centered value at any time by using the

6 formula:

7
$$f_N = Q_N \left(\frac{V_{MICRO}}{V_{MACRO}} \right),$$

8 wherein Q_N is the number of microgrid cells occupied by material N, V_{MICRO} is

9 the volume of a single microcell and V_{MACRO} is the volume of a single control

10 volume.

11

12 Given the example of FIG. 2, and assuming evenly distributed microgrid cells

13 in the 1 x 1 control volume, $f_1 = 5/16 = 0.3125$; $f_2 = 5/16 = 0.3125$ and $f_3 = 6/16$

14 $= 0.3750$.

15

16 Average volume centered values of density ρ and viscosity μ, for example,

17 in each control volume can then be recovered through:

18

19
$$\rho = \sum_N f_N \rho_N \text{ and } \mu = \sum_N f_N \mu_N \text{ respectively.}$$

20

21 In step 160, equations of fluid motion are solved for each of the macrogrid

22 control volumes to arrive at a velocity field for each of the control volumes (as

23 well as other conserved variables such as pressure, turbulent kinetic energy,

24 and temperature). The solution of these equations depends upon the volume

25 centered values of density ρ and viscosity μ for each of the control volumes

-11-

1 (or, in general, all fluid property variables). These equations rely upon

2 principles of conservation of mass, conservation of momentum, and

3 conservation of energy to derive velocity fields across each of the control

4 volumes during each time step of the simulation. More particularly, the

5 general equations of fluid motion include (written in tensor form):

6

7 $$\partial\rho/\partial t + \partial\rho u_i/\partial x_i = 0 \qquad \text{(continuity equation)}$$

8

9 $$\rho\, \partial u_i/\partial t + \rho u_j\, \partial u_i/\partial x_j = -\partial P/\partial x_i + \sigma_{ij} + \rho g_i \quad \text{(momentum equation)}$$

10

11 $$C_p\, \partial\rho T/\partial t + C_p\, \partial\rho u_i T/\partial x_i = \partial P/\partial t + u_i\, \partial P/\partial x_i + \partial/\partial x_i(k\, \partial T/\partial x_i) + \mu\Phi + Q$$

12 $$\text{(energy equation)}$$

13

14 where: u_i is the velocity is the i-coordinate direction, t is time, x_i is the spatial

15 coordinate in the i-direction, P is pressure, σ_{ij} is the strain rate tensor, C_p is

16 constant pressure specific heat, T is temperature, k is thermal conductivity, Φ

17 is viscous dissipation, and Q is internal heat sources.

18

19 For simulation purposes, these equations are discretized into algebraic

20 equations which are readily solved by iterative numerical techniques.

21 Specifically, the discretized conservation equations for all control volumes are

22 solved in an iterative manner. For example, when the x momentum equation

23 is solved, all other unknowns are fixed (such as y and z momentum (in the 3D

24 case), pressure, and density) to their most current iterative values, resulting in

25 the only unknown variable being the x momentum. The resulting set of linear

26 equations for the x momentum is then solved with a conjugate gradient type

27 method for example. The x momentum field is then updated and this process

28 is repeated for the y momentum, then z momentum, etc., working the iteration

29 through each unknown variable. At the end of the iterative loop, all unknowns

30 have effectively been updated to the next iteration level. This iterative cycle is

31 continued until a set of convergence criteria are achieved (based on residuals

32 and iterative value changes), and then the time step is complete and the

1   variable fields (velocity, pressure, temperature, etc.) are effectively updated to

2   the next time and the above procedure is repeated again for the next time

3   step. As a result of solving these equations, the velocity field (v_x, v_y, and v_z) in

4   each control volume is determined as well as all other flow field variables

5   (pressure, etc).

6

7   Those skilled in the art will appreciate that knowing the volume fractions, and

8   subsequently average volume centered values of density ρ and viscosity μ

9   for each of the control volumes (as well as all other flow field variables), many

10   different alternative solution schemes may be used to calculate the velocity

11   fields or other values needed in order to calculate movement of the microgrid

12   cells. The present invention provides the advantage that numerous different

13   fluids materials may be used in a simulation with the volume fractions of the

14   control volumes being readily calculated. From these volume fractions,

15   average parameters needed to solve equations of fluid motion can be readily

16   derived. Consequently, a wide number of methods or algorithms can be used

17   to estimate velocity fields or other variables which are useful in computational

18   fluid dynamic simulations. These parameters would then be used to advect or

19   move microgrid cells as will be described below.

20

21   Step 170 includes advecting the microgrid cells within the macrogrid and each

22   of the control volumes in accordance with the iterative velocity fields

23   calculated in step 160. This displacement of microgrid cells will result in some

24   of the microgrid cells overlapping one another in some of the microgrid

25   locations and other microgrid locations being left void. FIG. 4 illustrates such

26   a microgrid containing overlapping and void microgrid locations.

27

28   The microgrid cells move only as a complete unit and individually represent a

29   single material. A fundamental premise of the microgrid scheme is that a

30   material may not become less than 1 microgrid in size. The microgrid is the

31   fundamental length or volume scale in the simulation. Each microgrid cell

32   reacts to its associated local control volume or macrogrid velocity conditions

1   and may subsequently be displaced to another control volume after

2   movement is rectified.

3

4   Movement or displacement of a microgrid cell in a particular direction is

5   determined by the velocity field of the control volume in a particular direction

6   (x, y or z) and the duration of movement, i.e., the length of the time step. For

7   example, if the average velocity of a control volume in the x-direction, as

8   determined in step 160, is 0.5 meters/second and the duration of a time step

9   is 1 second, then each of the microgrid cells in that control volume would want

10   to be moved 0.5 meters along the x-direction. If the size of each microgrid

11   cell is 0.5 meters, then each microgrid cell in that particular control volume

12   would be displaced by one microgrid cell. Similarly, the microgrid cells in the

13   control volumes may also move in the y- and z- directions, if a 3 dimensional

14   model were used.

15

16   Movement of the microgrid cells is only allowed if the microgrid cell has

17   reached the threshold of moving at least one microgrid cell unit. In this

18   exemplary embodiment, when a microgrid cell experiences a velocity

19   condition too small to warrant movement, this information is flagged and the

20   next iteration step is performed and so on until movement is imminent based

21   on the local velocity field. If the velocity field is not of sufficient strength to

22   warrant movement of a microgrid cell, then it simply remains in its current

23   location. In this way, an accurate accounting of the effects of velocity can be

24   maintained while utilizing a somewhat coarse microgrid.

25

26   As the advection step begins, an interim array is used to receive advected

27   microgrid cell information. This interim array is initialized to values of "1", and

28   the size of the interim array corresponds to the size of the microgrid cellular

29   field. During the advection step, new microgrid cell values are constructed via

30   a multiplicative association of primes and then stored in the interim array at

31   the appropriate locations. For example, a microgrid cell receiving one copy of

32   a single material (such as material 1) would be represented by 1 x 43 = 43. A

1   microgrid cell receiving 2 different materials may be numerically represented

2   as 1 x 43 x 53 = 2279, which indicates the presence of both materials 1 and 3

3   in the microgrid cell. Similarly, a cell may receive two copies of the same

4   material (e.g. 1 x 43 x 43 = 1849). If no material is advected into an interim

5   array location, then the value remains as "1" and indicates that void is

6   present. Again, FIG. 4A illustrates the spatial distribution of prime numbers in

7   a macrogrid after the advection step 170 is complete. (Note that the original

8   distribution of microcell fluid materials before the advection step is shown in

9   FIG. 3.) Where there is a void, the array contains a numeral "1". Where there

10   is an overlap of microgrid cells, the product of the material identifers (primes)

11   of the overlapping microgrid cells is given.

12

13   After every iteration within a time step the microgrid cells must be reallocated,

14   step 180, so that there are no remaining overlapping cells or voids in the

15   microgrid. Microgrid locations that contain more than one identifying prime

16   number or material must be stripped to a single prime number with the other

17   identifiers shifted to new locations. Microgrid locations void of any prime

18   identifier must be filled. The reallocation scheme preferably is designed to

19   achieve the objectives of insuring conservation of variable fields (mass,

20   momentum, and energy).

21

22   A correction algorithm is designed to detect values that are larger than the

23   largest prime in the system, which are representative of overlaps of microgrid

24   cells. These few numbers are then evaluated to ascertain the contents of the

25   associated microgrid cells. By controlling what primes are available to create

26   interim microgrid cell values, the evaluation of overlapping and void microgrid

27   spaces is reduced to a single greater than or less than comparison.

28   Consequently, when a large number is detected, the possible factors of that

29   number are contained in a small subset of the known primes. Specifically,

30   these are the primes created by the Eulerian quadratic generator, p(N),

31   defined in Table 1. All together, this technique greatly reduces the

1   computational cost to evaluate the contents and reorganization of microgrid

2   cells.

3

4   For example, given the numeric representation in FIG. 4B, the algorithm

5   detects that the number 2279 is larger than the largest prime in the system

6   (which in this case is 53) and begins a scheme that delineates the contents of

7   the cell, breaking the integer 2279 into its prime components that represent

8   the materials therein. Specifically, the algorithm exploits the concept of

9   modular arithmetic until a solution of 0 is calculated. Recall from the rules of

10   modular arithmetic that $(2279 \bmod 53) = 43$. And, $(43 \bmod 43) = 0$.

11

12   A preferred exemplary reallocation procedure is described in Flowchart 2 of

13   FIG. 6. Again, those skilled in the art will realize that many other alternative

14   reallocation procedures or algorithm could be used to rearrange the

15   overlapping microgrid cells and voids to establish a microgrid having a single

16   fluid material or microcell in each microgrid location, as was the case in the

17   initial microgrid cell arrangement shown in FIG. 3. The different reallocation

18   procedures can be used to achieve different reallocation objectives such as

19   using subiterations to balance material distributions.

20

21   The first step 220 in FIG. 6 is to scan the entire microgrid field for "1" 's or

22   void locations. Recall that the temporary grid that holds the transported or

23   fluxed identifiers (primes) is initialized with 1's. If no primes flux into a

24   microgrid location, the value "1" is maintained. These locations correspond to

25   a microcellular void and a sum of their number gives a maximum number of

26   overlap sites that subsequently sizes a caching array. It is possible that a

27   single location may hold more than one overlap so void locations may

28   outnumber overlapped locations. The caching array is used to record excess

29   or stripped identifiers from microgrid cells during the reallocation process.

30

31   Next in step 230, the microgrid is scanned for microgrid cells that contain

32   overlapped single materials. These are locations that contain multiple copies

1   of the same prime number. In this situation, the excess primes are stripped

2   (step 240) from the microgrid cells using modular arithmetic and then placed

3   into the caching array, while one copy is left behind to fill the location.

4   Mathematically, the following evaluation occurs:

5

6 $$\text{If: } f > p(N_{max}) \text{ and } MOD(f, p(N)) = 0 \text{ where}$$

7 $$f > p(N), \; p(N) = N^2 + N + 41, \text{and } f, N \in Z^+,$$

8 $$N = \{N_1, N_2, N_3, ..., N_{max}\}.$$

9   then there are multiple copies of the same prime (or material).

10   In step 250, subsequently the "1" 's locations are quickly evaluated against

11   their gradient condition. The gradient condition is evaluated by solving $\nabla f_N =$

12   0 . The bulk void is filled using available primes from the caching array by

13   evaluating the gradient condition (in 2D or 3D space). This means that if all

14   the microgrid cells in closest proximity (i.e. every touching microgrid cell) are

15   the exact same prime number, and there is an equal prime number available

16   in the caching array, the "1" is immediately replaced with the corresponding

17   prime. This reduces the number of locations that must be evaluated in a

18   conservation of mass routine, to be described below.

19

20   At this point the microgrid system may still contain overlaps that hold different

21   primes as well as still having void or "1" locations. The "1" locations typically

22   develop at interfaces, grid edges, or in areas of large scale (relative to the

23   mesh) bulk motion. The overlaps are all interfacial areas.

24

25   Once again, the microgrid is scanned for cells that contain more than one

26   prime (or different materials). This is done in step 260 by exploiting the

27   property of the Eulerian generator, $p(N) = N^2 + N + 41$ ($N = 1,2,..39$), such that

28   the smallest prime squared is larger than the largest prime.

29 $$\text{If: } f > p(N_{max}) \text{ and } MOD(f, p(N)) > 0 \text{ where}$$

30 $$f > p(N), p(N) = N^2 + N + 41, \text{and } f, N \in Z^+,$$

31 $$N = \{N_1, N_2, N_3, ..., N_{max}\}. \text{ then,}$$

1

2   these locations correspond to microgrid cells with interfacial overlap.

3

4   When these cells are located, all of the prime identifiers are removed from the

5   location. An evaluation is made as to which prime most appropriately fills the

6   location. This is done by an evaluation of local fluid fraction gradient and a

7   momentum value assigned to each material based on the local velocity

8   condition. More particularly, the overlapped cells are evaluated based on

9   gradient, ∇f_N and momentum, $\rho_N |v|$, criteria, such that a physical motivation

10   is established to identify the correct material distribution. The most ideal

11   candidates for primes are chosen and the excess primes are stripped to the

12   caching array.

13

14   Once all of the overlaps are corrected, all that is left are microgrid cellular

15   locations that contain a "1" and the remaining material identifiers in the

16   caching array. In step, 280, the remaining voids are evaluated using

17   maximum material gradient condition, momentum considerations and material

18   content of the caching array. Ideally, a particular material or prime is selected

19   such that its reallocation provides a maximum or optimal gradient condition.

20   Mathematically, this means that p_N, such that min (∇f_N) for N = 1, 2, 3,…. This

21   choice of material is preferably overridden if a microcell exceeds a

22   predetermined momentum criteria, i.e. momentum = mass of microcell x

23   velocity which is greater than a predetermined threshold for momentum. If so,

24   the high momentum microgrid cell(s) are located in the void. In this way,

25   individual high momentum microcells are allowed to "pierce" otherwise

26   continuous flows of other materials.

27

28   FIG. 7 shows a third flowchart which summarizes step 280 used in evaluating

29   and filling these remaining voids. In step 320, the microgrid voids are

30   evaluated for maximum gradient condition. More specifically, the maximum

31   gradient condition is evaluated by scanning linearly for locally dissimilar

32   material as described in step 330a. FIG. 5A illustrates that from a particular

1   starting "S" void location, neighboring microgrid cells are scanned in 8 linear

2   directions. The scan begins in the direction with the greatest gradient. If the

3   prime selected is available in the caching array, a replacement is made in the

4   particular void.

5

6   In step 340a, the needed prime is extracted from its closest neighbor and is

7   replaced with a prime from the caching array. In step, 350a the void is

8   replaced with the just extracted prime.

9

10 If a desired prime is not available in the caching array, a scan, step 330b, is

11 made starting from the particular microgrid void or starting position "S" and

12 moving out in every linear direction (8 in 2D, 26 in 3D) where an attempt is

13 made to find the prime locally. Once found, the microgrid is adjusted in that

14 direction to compensate for a material imbalanced distribution. In step 340b,

15 the needed prime from the closest neighbor is extracted and a void is created

16 in a new location. The original void is then replaced with the extracted prime,

17 step 350b. The 'new' void is then evaluated for maximum gradient condition

18 in step 360b. In step 370b, the grid is scanned linearly from a new void area

19 for local dissimilar material that already exists in the caching array. Steps

20 330a, 330b and 330c are then repeated.

21

22 Step 330c provides a procedure to address the issue of an unsuccessful grid

23 scan for dissimilar materials. Using a randomizer, the starting location for the

24 scan is moved in step 340c. In step 350c, the contents of microgrid cells are

25 exchanged. Again the steps may be taken as described in steps 330a, 330b

26 or 330c.

27

28 Usually what results is a slight local reorganization that conserves mass. If

29 this is not possible, a mass error is accrued and through the progress of a

30 calculation, the total mass error is determined and used as a gauge to

31 evaluate the overall simulation accuracy.

32

1   Once broken down, a separate algorithm, described in Flowchart 3 of FIG. 6

2   evaluates the local condition ∇f_N for each N and designates the best

3   candidate prime for the previously overlapped microgrid cell. The prime NOT

4   replaced in the once mixed cell is then redistributed to a next best location.

5   Ideally, this location is the closest cell in the direction of its strongest material

6   gradient. The algorithm is designed to scan in this direction in search of an

7   empty cell that will be best filled by the prime. If no such cell can be found, in

8   2D, 8 directions are scanned as shown in FIG. 5A. If still no candidate can be

9   located, the initial search is abandoned.

10

11   A small adjustment to the starting location of the search is made and the

12   multi-directional scan is resumed (see FIG. 5B). The user can define how

13   many times these small adjustments will be tolerated before an "interfacial

14   bump", for lack of a better description, is implemented. What happens is this:

15   the direction associated with the largest material gradient is rescanned for a

16   closest interface. At the interface, a material exchange is made, replacing the

17   closest interfacial cell with the local material at hand and then using this

18   location as a starting point to seek out a new site for the material that was

19   displaced, using the original searching algorithm. After several iterations of

20   this sequence, all empty microgrid cells and overlaps are corrected.

21

22   If sufficient iteration steps have occurred to achieve convergence, the

23   iteration is ended. If additional time steps are required, then step 150 is

24   repeated using the reallocated cells and their primes from step 180 to

25   redetermine the volume fractions in each of the control volumes. Steps 160-

26   190 are repeated until it is determined that sufficient time steps have occurred

27   and the simulation is ended in step 200.

28

29   <u>Computational Example 1</u>.

30

31   Circulating rectangular cavity flow offers a rigorously investigated,

32   complicated flow pattern for the reader's review. In this example, the cavity is

1   initialized with a stratified pattern of three similar materials, differing only in

2   prime designation not material properties. In this manner the similarity of the

3   flow form is qualified by literature comparison to a single fluid flow, as well as

4   to illustrate the use of three numerically distinct materials in the microgrid

5   algorithm.

6

7   Rhee et. al. (1984) and Freitas (1986) describe a similar recirculating cavity

8   flow such that given the schematic of FIG. 8, a plate drives a continuous

9   shear motion from front to back at the top of the cavity. FIG. 8 also illustrates

10   the formation of secondary eddies in three of the four corners of the cavity

11   along a center plane. FIG. 9 is a photograph of Rhee's experimental flow

12   along a similar plane for comparison. FIG. 10 is a rendering of the microgrid

13   algorithm output for the three stratified materials described in the previous

14   paragraph.

15

16   As shown in FIG. 10, clearly a portion of the bottom layer is trapped in the

17   lower two eddies, while the balance of the material travels through the

18   recirculation pattern. The middle layer is most heavily mixed as it is quickly

19   taken up in the primary circulation cell then partially fragmented as it makes

20   its first full rotation. The top layer is partially trapped in the upper left hand

21   corner eddy with the balance following the primary circulation cell. It is

22   obvious that the microgrid algorithm is correctly capturing the proper features

23   of the recirculating cavity flow physically documented in FIG. 9 by Rhee et. al

24   (1984) and computationally rendered by Freitas (1986), while simultaneously

25   tracking three numerically separate materials.

26

27   To capture this refined detail, the simulation employs a fairly coarse mesh.

28   The physical dimension of the cavity portrayed in FIG. 10 is 150 mm x 150

29   mm. The computational macrogrid is 126 x 126. The microgrid cell mesh is 4

30   x 4. Numerical experiments verify that an increase in microgrid mesh while

31   maintaining the original computational mesh yields more refined results with a

32   minimal increase in computational expense.

1

2   EXAMPLE 2

3

4   As an example, this same simulation is offered with 126 x 126 computational

5   mesh and a microgrid cell mesh of 2 x 2 (1/4 of the microgrid resolution

6   shown in the above simulation of FIG. 10) in a side by side comparison at

7   time step =210. This time step is chosen because it shows adequate detail of

8   all the eddy features.

9

10   Because the algorithm employs an additive and collective response measure

11   to the effect of velocity over multiple time steps, the more coarse the microgrid

12   cell refinement is, the less immediate physical response one can see in areas

13   of relatively low velocity. Similarly, because of the block-like movement of

14   microgrid cells, to capture areas of high thinning, microgrid cell size must be

15   reduced. This is most evident in the middle layer, where material should form

16   thin trails in response to the shear motion of the primary circulation cell. Also,

17   while the overall response of the system at coarse micromesh is good, it may

18   be noted that interfacial smoothness and subtle feature resolution is increased

19   with the refinement of the microgrid. It is important, however, to realize that at

20   no time is the computational mesh adjusted. These calculations are coupled

21   to the microgrid via a fluid fraction value only, and the computational mesh is

22   completely independent of microgrid cell size. The best computational value,

23   therefore, utilizes a coarse computational mesh with a refined microgrid mesh.

24

25   As the only algorithmic limitation of the microgrid process demonstrated here

26   with $p(N) = N^2 + N + 41$ is a numerical cap of 39 materials, it can easily be

27   demonstrate that the simulation methodology can be used with a larger

28   number of materials. Of course, the computational grid selection must be

29   chosen with prudence. Just as in a 2 material simulation, it is not wise to

30   represent a single material over too few computational cells.

31

32

1   EXAMPLE 3

2

3   The results shown in FIG. 12 utilize a 126 x 126 computational mesh with an

4   8x8 microgrid mesh. FIG. 13 is an artistic rendering of the 6 materials in the

5   same view at time step =120.

6

7   While in the foregoing specification this invention has been described in

8   relation to certain preferred embodiments thereof, and many details have

9   been set forth for purposes of illustration, it will be apparent to those skilled in

10   the art that the invention is susceptible to alteration and that certain other

11   details described herein can vary considerably without departing from the

12   basic principles of the invention.

13

14   **REFERENCES**

15

16   Daly, B.J., 1969, A technique for including surface tension effects in

17   hydrodynamic calculations. Journal of Computational Physics, Vol. 4, p. 97-

18   117.

19

20   Takizawa, A., Koshizuka, S., and Kondo, S., 1992, Generalization of physical

21   component boundary fitted co-ordinate (PCBFC) method for the analysis of

22   free-surface flow. International Journal of Numerical Methods in Fluids, Vol.

23   15, p. 1213-1237.

24

25   Sussman, M., Smereka, P. and Osher, S., 1994, A level set approach for

26   computing solutions to incompressible two-phase flow. Journal of

27   Computational Physics, Vol. 114, p. 146-159.

28

29   Osher, S. and Sethian, J.A., 1988, Fronts propagating with curvature-

30   dependant speed: algorithms based on Hamilton-Jacobi formulations.

31   Journal of Computational Physics, Vol. 79, p. 12-49.

32

1   Sethian, J.A., 1996, Level set methods: Evolving interfaces in geometry, fluid
2   mechanics, computer vision and materials sciences. Cambridge University
3   Press.
4
5   Nichols, B.D. and Hirt, C.W., 1973, Calculating three-dimensional free surface
6   flows in the vicinity of submerged and exposed structures. Journal of
7   Computational Physics, Vol. 12, p. 234-246.
8
9   Harlow, F.H. and Welch, J.E., 1965, Numerical calculation of time-dependent
10   viscous incompressible flow of fluid with free surface. Physics of Fluids, Vol.
11   8(12), p. 2182-2189.
12
13   Hirt, C.W. and Nichols, B.D., 1981, Volume of fluid (VOF) method for the
14   dynamics of free boundaries. Journal of Computational Physics, Vol. 39,
15   p.201-225.
16
17   Ashgriz, N. and Poo, J.Y., 1991, FLAIR: Flux line-segment model for
18   advection and interface reconstruction. Journal of Computational Physics,
19   Vol. 93, p. 449-468.
20
21   LaFaurie, B., Nardone, C., Scardovelli, R., Zaleski, S., and Zanetti, G., 1994,
22   Modeling merging and fragmentation in multiphase flows with SURFER.
23   Journal of Computational Physics, Vol. 113, p. 134-147.
24
25   Noh, W.F. and Woodward, P., 1976, SLIC (Simple Line Interface
26   Calculations). Lecture Notes in Physics, Vol. 59, p. 330-340.
27
28   Youngs, D.L., 1982, Time-dependent multi-material flow with large fluid
29   distortion. (in) Morton, K.W. and Baines, M.J. (eds) Numerical Methods for
30   fluid dynamics. London: Academic Press. p. 273-285.
31

1   Rider, W.J. and Kothe, D.B., 1998, Reconstructing volume tracking. Journal
2   of Computational Physics, Vol. 141, p. 112-152.

3

4   Gueyffier, D., Li, J., Nadim, A., Scardovelli, R. and Zaleski, S., 1999, Volume-
5   of-fluid interface tracking with smoothed surface stress methods for three-
6   dimensional flows. Journal of Computational Physics, Vol. 152, p. 423-456.

7

8   Scardovelli, R. and Zaleski, S., 2000, Analytical relations connecting linear
9   interfaces and volume fractions in rectangular grids. Journal of Computational
10 Physics, Vol. 164, p. 228-237.

11

12 Scardovelli, R., Aulisa, E., Manservisi, S., and Marra, V., 2002, A marker-VOF
13 algorithm for incompressible flows with interfaces. Proceedings of ASME
14 FEDSM'02, ASME 2002 Fluids Engineering Division Summer Meeting,
15 Montreal, Quebec, Canada, FEDSM2002-31241, p. 1-6.

16

17 Tomiyama, A., Nakahara, Y., and Abe, S., 2002, An interface tracking method
18 based on volume tracking in embedded micro cells. Proceedings of ASME
19 FEDSM'02, AMSE 2002 Fluids Engineering Division Summer Meeting,
20 Montreal, Quebec, Canada, FEDSM2002-31147, p. 1-6.

21

22 Rhee, H.S., Koseff, J.R., and Street, R.L., 1984, Flow visualization of a
23 recirculating flow by rheoscopic liquid and liquid crystal technique.
24 Experiments in Fluids, p. 57-64.

25

26 Freitas, C.J., 1986, Nonlinear transient phenomena in a three-dimensional
27 cavity flow: A numerical investigation. PhD dissertation, Stanford University.